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Rigorous results on superconducting ground states for attractive extended Hubbard models

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We show that the exact ground state for a class of extended Hubbard models including bond-charge, exchange, and pair-hopping terms, is the Yang “ η -paired” state for any nonvanishing positive value of the pair-hopping amplitude, at least when the on-site Coulomb interaction is attractive enough and the remaining physical parameters satisfy a single constraint. The ground state is thus rigorously superconducting. Our result holds on a bipartite lattice in any dimension, at any band filling, and for arbitrary electron hopping.

Interest in itinerant, strongly interacting electron systems has exploded since the discovery of high- T_c superconductors, for which the interplay between itinerant magnetism and insulating behavior is believed to play a crucial role. The Hubbard model¹ provides the simplest description of such systems, by assuming that the itinerant electrons interact only via an on-site term, and it has therefore been intensively studied. The original Bethe ansatz solution of the one-dimensional (1D) model at half-filling² has in recent years been supplemented by a number of additional rigorous results (see Ref. 3 for a current review). For instance, for the attractive (i.e., “negative U ”) Hubbard model, long studied as a model believed to have a superconducting ground state,⁴ recent articles have established the existence of “off-diagonal long-range order” [ODLRO (Ref. 5)], but these results have been restricted either to $U \rightarrow -\infty$ (Ref. 6) or to bipartite lattices in which the number of sites on one sublattice is not equal to that on the other.^{7,8,3} Indeed, although it is known⁹ that the Hubbard Hamiltonian has certain eigenstates (the “ η -paired” states) that have nonzero pairing and ODLRO and hence are superconducting, Yang has shown that these states can never be the ground state for the pure Hubbard model on a standard bipartite lattice.⁹

Apart from the Hubbard model itself, “extended” Hubbard models have also attracted considerable recent interest, in part because it has been recognized^{10,11} that the additional interaction terms (discussed but eventually neglected in the original papers¹) could be relevant in stabilizing some novel (e.g., ferromagnetic or superconducting) phases. For instance, Strack and Vollhardt¹² proved rigorously that the ground state for a class of extended Hubbard models is a saturated ferromagnet at half-filling for *any* nonvanishing positive value of the exchange term, provided that the Coulomb repulsion is strong enough.

In this paper we show that in appropriate regions of the parameter space of a class of extended Hubbard models, the superconducting phase is the stable ground state for *any* nonvanishing positive value of the pair-hopping term.^{10,13} More precisely, by simultaneous use of Yang’s states and of a suitable generalization of Strack and Vollhardt’s techniques, we prove rigorously that the ground state of the extended Hub-

bard model at any band filling and for average magnetization $m=0$ is superconducting, provided that the on-site Coulomb interaction is attractive enough and that the remaining physical parameters satisfy a single reasonable constraint. Moreover—after showing that at $X=0$ our model exhibits the full $SO(4)$ dynamical algebra characteristic of the conventional Hubbard model—by means of a particle-hole transformation we map the result at $X=0$ into a sufficient criterion for stability of ferromagnetism in the repulsive case at half-filling and for arbitrary m , which criterion is more general than the one given in Ref. 12. Importantly, in contrast to other recent work,^{14–16} the supersymmetric condition $t=X$ [see (1) below] is in general neither required nor fulfilled by our superconducting ground state.

Our extended Hubbard Hamiltonian reads¹

$$\begin{aligned}
 H = & -t \sum_{\langle j,k \rangle} \sum_{\sigma} c_{j,\sigma}^{\dagger} c_{k,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow} \\
 & + X \sum_{\langle j,k \rangle} \sum_{\sigma} (n_{j,-\sigma} + n_{k,-\sigma}) c_{j,\sigma}^{\dagger} c_{k,\sigma} + \frac{V}{2} \sum_{\langle j,k \rangle} n_j n_k \\
 & + \frac{W}{2} \sum_{\langle j,k \rangle} \sum_{\sigma, \sigma'} c_{j,\sigma}^{\dagger} c_{k,\sigma'}^{\dagger} c_{j,\sigma'} c_{k,\sigma} \\
 & + \frac{Y}{2} \sum_{\langle j,k \rangle} \sum_{\sigma} c_{j,\sigma}^{\dagger} c_{j,-\sigma}^{\dagger} c_{k,-\sigma} c_{k,\sigma}, \quad (1)
 \end{aligned}$$

where $c_{j,\sigma}^{\dagger}, c_{j,\sigma}$ are fermionic creation and annihilation operators ($\{c_{j,\sigma'}, c_{k,\sigma}\} = 0$, $\{c_{j,\sigma}, c_{k,\sigma'}^{\dagger}\} = \delta_{j,k} \delta_{\sigma,\sigma'} \Pi$, $n_{j,\sigma} \doteq c_{j,\sigma}^{\dagger} c_{j,\sigma}$, $n_j = \sum_{\sigma} n_{j,\sigma}$) on a d -dimensional lattice Λ ($j, k \in \Lambda$, $\sigma \in \{\uparrow, \downarrow\}$), and $\langle j,k \rangle$ stands for nearest neighbors (NN) in Λ . In (1) the first term represents the band energy of the electrons, and the remaining terms describe their Coulomb interaction energy in a narrow band approximation:¹ U parametrizes the on-site diagonal interaction, V the neighboring site charge interaction, X the bond-charge interaction, W the exchange term, and Y the pair-hopping term. An explicit evaluation of the relative size of these contributions—all generated from on-site and NN matrix elements of the Coulomb interaction—was already given in Ref. 1. It is worth

emphasizing that most of the following analysis can be extended in a straightforward way to the case in which the interactions in (1) are not confined to neighboring sites. However, to avoid cumbersome notation, we have chosen to limit ourselves to the present case.

The exchange and pair-hopping terms in (1) can be written more conveniently in terms of the conventional spin and pseudospin operators $S_j^{(\alpha)}$ and $\tilde{S}_j^{(\alpha)}$, $\alpha = x, y, z$,

$$\begin{aligned} S_j^{(+)} &= c_{j,\uparrow}^\dagger c_{j,\downarrow}, \quad S_j^{(-)} = (S_j^{(+)})^\dagger, \quad S_j^{(z)} = \frac{1}{2}(n_{j,\uparrow} - n_{j,\downarrow}), \\ \tilde{S}_j^{(+)} &= (-)^{|j|} c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger, \quad \tilde{S}_j^{(-)} = (\tilde{S}_j^{(+)})^\dagger, \\ \tilde{S}_j^{(z)} &= \frac{1}{2}(n_{j,\uparrow} + n_{j,\downarrow} - 1), \quad S_j^{(\pm)} \doteq S_j^{(x)} \pm i S_j^{(y)}, \\ \tilde{S}_j^{(\pm)} &\doteq \tilde{S}_j^{(x)} \pm i \tilde{S}_j^{(y)}, \end{aligned} \quad (2)$$

which are known to generate two orthogonal $\text{su}(2)$ algebras. For a *bipartite* lattice with an even number of sites, the second line of (1) reads then

$$2V' \sum_{\langle j,k \rangle} \tilde{S}_j^{(z)} \tilde{S}_k^{(z)} - W \sum_{\langle j,k \rangle} \mathbf{S}_j \cdot \mathbf{S}_k - Y \sum_{\langle j,k \rangle} \tilde{\mathbf{S}}_j \cdot \tilde{\mathbf{S}}_k + C, \quad (3)$$

where $V' = V - (1/2)(W - Y)$ and $C = (1/2)(V - W/2)qN(2n - 1)$, with q the number of nearest neighbors in Λ , N the number of sites, and n the average electron number per site.

H can be easily seen to commute with $\text{su}(2)_f$, generated by $S_\alpha = \sum_j S_j^\alpha$, $\alpha = x, y, z$. This observation is in fact relevant in recognizing the $(N+1)$ -fold degenerate saturated ferromagnetic state $|\psi_m\rangle$,

$$|\psi_m\rangle \doteq (S_+)^{(n+m)N/2} |\downarrow \downarrow \cdots \downarrow\rangle, \quad |m| \leq \min\{1, n\}, \quad (4)$$

as eigenstate of H at $n=1$ (half-filling) and average magnetization per site m . Analogously, one can construct $\text{su}(2)_{sc}$, generated by $\tilde{S}_\alpha = \sum_j \tilde{S}_j^\alpha$. The latter does not commute with H . Nevertheless, it is easily checked that the states, known as η pairs,⁹ defined by

$$|\eta_n\rangle \doteq (\tilde{S}_+)^{nN/2} |0\rangle, \quad 0 \leq n \leq 2, \quad (5)$$

with $|0\rangle$ being the electron vacuum, are eigenstates of H at band filling n with $m=0$, provided that $V'=0$. Interestingly enough, these states are precisely those which Yang has proved to exhibit ODLRO, which property has been shown to imply both the Meissner effect and flux quantization,¹⁷ i.e., superconductivity. Notice that the η pairs (5) differ from the pairs defined in Ref. 16 by a factor of $(-)^{|j|}$; this will be essential in the following.

Assuming henceforth $V'=0$, we want to investigate under which circumstances $|\eta_n\rangle$ is indeed the ground state. We proceed by rewriting, by means of suitable operator identities, the hopping and bond-charge repulsion terms as sums of positive definite operators having zero eigenvalue on (5) plus contributions which simply renormalize the other terms in the Hamiltonian, which now reads

$$\begin{aligned} H &= -U' \sum_j [S_j^{(z)}]^2 - W' \sum_{\langle j,k \rangle} \mathbf{S}_j \cdot \mathbf{S}_k - Y' \sum_{\langle j,k \rangle} \left(\tilde{\mathbf{S}}_j \cdot \tilde{\mathbf{S}}_k - \frac{1}{4} \right) \\ &\quad + J \sum_{\langle j,k \rangle} S_j^{(z)} S_k^{(z)} + C' \\ &\quad + \sum_{\langle j,k \rangle} \left\{ |t-X| |\gamma| O_{jk}^\dagger O_{jk} + \sum_\sigma [|t-X| |1-\gamma| P_{jk,\sigma}^\dagger P_{jk,\sigma} \right. \\ &\quad \left. + |X| (Q_{jk,\sigma} Q_{jk,\sigma}^\dagger + R_{jk,\sigma}^\dagger R_{jk,\sigma}) \right\}, \end{aligned} \quad (6)$$

where $U' = 2\{U + q[|t-X|(\gamma\alpha^2 + |1-\gamma|\beta^2) + 4|X|]\}$, $W' = W - \beta^2|t-X||1-\gamma|$, $Y' = Y - |t-X|[2|\gamma/\alpha^2 + |1-\gamma|\beta^2|]$, $J = |t-X|[2|\gamma|(\alpha^2 + 1/\alpha^2) - |1-\gamma|(\beta^2 + 1/\beta^2)]$, and $C' = C - (1/2)(Un + Yq/2)N$. Here $\alpha \neq 0$, $\beta \neq 0$, and γ are free parameters, and

$$\begin{aligned} O_{jk} &= \alpha(S_j^{(z)} - S_k^{(z)}) + \frac{\epsilon}{\alpha}(c_{k,\uparrow}^\dagger c_{j,\uparrow} + c_{j,\downarrow}^\dagger c_{k,\downarrow}), \\ P_{jk,\sigma} &= \frac{1}{2} \left[\beta(S_j^{(\sigma)} - S_k^{(\sigma)}) + \frac{\eta}{\beta}(c_{k,\sigma}^\dagger c_{j,-\sigma} - c_{j,\sigma}^\dagger c_{k,-\sigma}) \right], \\ Q_{jk,\sigma} &= \frac{1}{\sqrt{2}}(n_{j,-\sigma} c_{j,\sigma} + \theta n_{k,-\sigma} c_{k,\sigma}), \\ R_{jk,\sigma} &= \frac{1}{\sqrt{2}}[(1 - n_{j,-\sigma})c_{j,\sigma} + \theta(1 - n_{k,-\sigma})c_{k,\sigma}], \end{aligned} \quad (7)$$

with $\epsilon = \text{sgn}[(t-X)\gamma]$, $\eta = \text{sgn}[(t-X)(1-\gamma)]$, and $\theta = \text{sgn}[X]$.

For $U' \leq 0$ and $Y' \geq 0$ the lower bound of the on-site and pair-hopping terms in (6) is zero, which coincides with their eigenvalue on the states $|\eta_n\rangle$. Moreover,

$$O_{jk}|\eta_n\rangle = P_{jk,\sigma}|\eta_n\rangle = Q_{jk,\sigma}^\dagger|\eta_n\rangle = R_{jk,\sigma}|\eta_n\rangle = 0, \quad (8)$$

and, H being a positive definite form in these operators, $|\eta_n\rangle$ is the ground state also for the second line of (6). The freedom in the choice of α , β , and γ permits two of them to be fixed so that $W'=0=J$. In this case, one finds that the state $|\eta_n\rangle$ is the ground state with energy $E_{g.s.} = (1/2) \times (U - qY)nN$ whenever $U' \leq 0$, and $Y' \geq 0$. In fact, we can obtain an even larger region of values of U for which $|\eta_n\rangle$ is the ground state if, instead of fixing α , β , and γ as above, we first express both the Ising-like term and the ferromagnetic exchange term in (6) through the following operator identities,

$$\begin{aligned} -W' \sum_{\langle j,k \rangle} \mathbf{S}_j \cdot \mathbf{S}_k &= |W'| \left(\sum_{\langle j,k \rangle} B_{jk}^\dagger B_{jk} - 2q \sum_j [S_j^{(z)}]^2 \right) \\ &\quad - W' \sum_{\langle j,k \rangle} S_j^{(z)} S_k^{(z)} J' \sum_{\langle j,k \rangle} S_j^{(z)} S_k^{(z)} \\ &= |J'| \left(\frac{1}{2} \sum_{\langle j,k \rangle} [S_j^{(z)} + \text{sgn}(J') S_k^{(z)}]^2 \right. \\ &\quad \left. - q \sum_j [S_j^{(z)}]^2 \right), \end{aligned} \quad (9)$$

with

$$B_{jk} = \frac{1}{\sqrt{2}} [c_{j,\uparrow}^\dagger c_{j,\downarrow} - \text{sgn}(W') c_{k,\uparrow}^\dagger c_{k,\downarrow}], \quad (10)$$

and $J' = J - W'$. The identities (9) when inserted in (6) further renormalize the coefficient of the Coulomb interaction term (i.e., $\sum_j [S_j^{(z)}]^2$), so that the inequalities which have to be satisfied in order that $|\eta_n\rangle$ be the ground state now read

$$U' + q(2|W'| + |J'|) \leq 0, \quad Y' \geq 0, \quad (11)$$

and are still functions of α , β , and γ . Eliminating α using the second equation of Eqs. (11), one is left with a single inequality for $u \equiv U/qt$,

$$u \leq - \left\{ 4x + |1-x| \left[\frac{2\gamma^2}{B} + \frac{(1-\gamma)^2}{\frac{y}{|1-x|} - B} \right] + \left| \frac{w}{|1-x|} - \frac{(1-\gamma)^2}{\frac{y}{|1-x|} - B} \right| + \left| \frac{2\gamma^2}{B} + B - \frac{w+y}{2|1-x|} \right| \right\}, \quad (12)$$

where x , y , and w are X , Y , and W expressed in units of t , and $B = y/|1-x| - |1-\gamma|/\beta^2$, $0 < B < y$. Equation (12) can be optimized by fixing the remaining parameters β (through B) and γ variationally. The result gives a *sufficient* condition for the superconducting state $|\eta_n\rangle$ to be stable ground state. This ground state is *unique* for $Y' > 0$, for in that case it is the unique ground state of the pair-hopping term in (6). The constraint $V' = 0$ [i.e., $V = (1/2)(W - Y)$] must be satisfied. The above rigorous result holds for any bipartite lattice, in any dimension, and importantly for *arbitrary* values of x . In particular, for $v = x = y = w = 0$ one finds directly from (12) that the pure Hubbard model has a superconducting ground state with ODLRO at least for $u = -\infty$, in agreement with Ref. 6.

The final explicit form of the general result (12) is too long to be written in the present paper, and will be reported elsewhere.¹⁸ Here we simply plot in Fig. 1 the actual boundary of our rigorous superconducting region in the u -vs- y plane at different x values. The inequality (12) and Fig. 1 show that at *any* $y \neq 0$ there is a region of u values for which the system is superconducting, and its size increases with increasing y , at least for $y \leq |1-x|$. It is quite natural that a nonvanishing value of y can stabilize the superconducting phase, in that it removes the degeneracy of the expectation value of the Hamiltonian on states $|\Phi_n(\phi)\rangle = [\sum_j e^{i\phi \cdot j} (c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger)]^{n(N/2)}$, which, for arbitrary $\phi \neq \pi$ and $x \neq 1$, are not eigenstates of H . As pointed out by Yang in Ref. 9, this observation implies that $|\eta_n\rangle \equiv |\Phi_n(\pi)\rangle$ cannot possibly be the ground state at $y=0$. On the contrary, for $x=1$ and $y=0$, $|\Phi_n(\phi)\rangle$ is an eigenstate of H for all ϕ and can in principle be the (degenerate) ground state. Indeed, from (12) we see that this is the case at least for $u \leq -4$. For $y \neq 0$, $x \neq 1$, $\langle \Phi_n(\phi) | H | \Phi_n(\phi) \rangle$ becomes a function of ϕ , in fact minimized by $\phi = \pi$, and $|\Phi_n(\pi)\rangle$ turns out to be the ground state at least in the region of U values satisfying (12). Finally, for $x=1$ and $y \neq 0$, there are two choices of ϕ which correspond to eigenstates of H , $\phi = \pi$ [for

$V = (1/2)(W - Y)$] and $\phi = 0$ [for $V = (1/2)(W + Y) < 0$]. The first corresponds to the ground state at least for $u \leq -(4 + y + w)$ [see (12)], whereas the region of stability of the solution corresponding to the second was already discussed in Ref. 16.

The relation (12) has a solution only for negative values of u . On the other hand, the physics of high- T_c materials suggests that the actual value of the on-site electron interaction is strongly repulsive. Even if the electron-phonon coupling reduces the effective value of the Hubbard interaction,¹⁹ its sign is still expected to be positive. However, one should keep in mind two points. First, (12) is a *sufficient* condition, and thus does not eliminate the possibility of having $|\eta_n\rangle$ as ground state even when it is not fulfilled. Again, the easier case $x=1$ helps clarify this point. There, an exact solution in 1D (Ref. 20) shows that ODLRO and superconductivity still survive as part of the degenerate ground state up to moderately positive values of u , which values are now band-filling dependent. We thus expect this behavior to persist even when the condition $x=1$ is relaxed. In particular, it would be extremely interesting to work out an exact Bethe ansatz solution of (1) in $d=1$, at least at $x=0$ (for $u=w=0$ the latter would be the superconducting “ $t-Y$ ” model, which is the particle-hole transformation of the *ferromagnetic* $t-J$ model²¹). Second, and very importantly, knowing rigorously both the superconducting nature of the ground state and its explicit form in any dimension provides powerful benchmarks for the approximate methods required to examine more realistic models.

Apart from the superconducting solution, our expression (6) for H allows us also to recognize a region of the parameter space characterized by ferromagnetic order. Indeed, it is easily seen that the state $|\psi_m\rangle$ of (4) can be obtained from the state $|\eta_n\rangle$ of (5) by the following unitary particle-hole transformation:

$$c_{j,\uparrow} \rightarrow c_{j,\uparrow}, \quad c_{j,\downarrow}^\dagger \rightarrow (-)^{|j|} c_{j,\downarrow}. \quad (13)$$

The same transformation maps $S_j^{(\alpha)}$ into $\tilde{S}_j^{(\alpha)}$, and the consequences for H as given by (6) can be worked out directly. Let us call the transformed Hamiltonian \tilde{H} . For $X=0$, \tilde{H} is still an extended Hubbard model, in which the on-site Coulomb repulsion term has opposite sign, W and Y have exchanged their roles (the first becoming the pair-hopping amplitude, and the second the exchange coupling), and the operators of (7)–(10) have been redefined accordingly. Moreover, an arbitrary neighboring-site Coulomb repulsion term can be added to \tilde{H} , as now it simply renormalizes the coefficient J of the Ising-like term in (6). The discussion following (6) can be used to examine the conditions under which the saturated ferromagnetic state $|\psi_m\rangle$ is the ground state of \tilde{H} . A straightforward calculation shows that the result is identical (in form) to the one given in (12), apart from the sign of u , the inequality hence becoming a lower bound for positive u . Further, now it is the exchange coupling which cannot be zero in order to have a stable ferromagnetic phase. This result is in full agreement with Ref. 12. In fact, our lower bound can easily be seen to coincide with expression (6) of Ref. 12 for $\gamma=0$, whereas it is lower than that if γ is fixed variationally. Again, a more complete discussion of

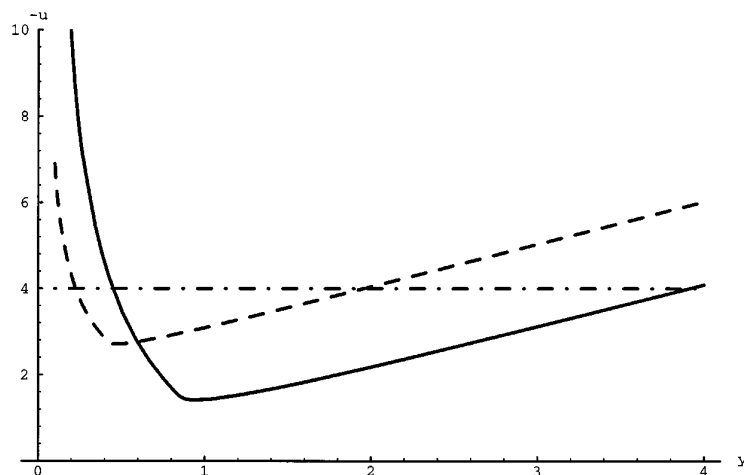


FIG. 1. The boundary of the superconducting phase in the $-u$ - y plane for different x values, $x=0, 0.5, 1$ (represented by solid, dashed, and dot-dashed lines, respectively), for $v=0$, $w=y$.

this case will be given elsewhere.¹⁸ Notice that in Ref. 12 the ‘freedom in the polarization of the saturated ferromagnet was not explicitly incorporated, which hid the power of the particle-hole transformation.

In summary, we have shown rigorously that a large class of extended Hubbard models on bipartite lattices has a superconducting ground state for negative U and nonvanishing pair-hopping amplitude. The conditions derived here are sufficient, depend in a trivial way on the dimension, and do not depend at all on the band filling. Of course, this does not exclude that a superconducting ground state can exist even

for moderate positive values of U . If this is the case, we expect that the dimension and the band filling should become crucial, as happens for instance in the $t=X$ case. Work is in progress along these lines.

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